

# The A-Cycle Problem for Transverse Ising Ring

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**Abstract.** Traditionally, the transverse Ising model is mapped to the fermionic c-cycle problem, which neglects the boundary effect due to thermodynamic limit. If persisting on a perfect periodic boundary condition, we can get a so-called a-cycle problem that has not been treated seriously so far (Lieb *et al.*, 1961 *Ann. of Phys.* **16** 407). In this work, we show a little surprising but exact result in this respect. We find the oddity of the number of lattice sites,  $N$ , in the a-cycle problem plays an unexpected role even in the thermodynamic limit,  $N \rightarrow \infty$ , due to the boundary constraint. We pay a special attention to the system with  $N(\in \text{Odd}) \rightarrow \infty$ , which is in contrast to the one with  $N(\in \text{Even}) \rightarrow \infty$ , because the former suffers a ring frustration. As a new effect, we find the ring frustration induces a low-energy gapless spectrum above the ground state. By proving a theorem for a new type of Toeplitz determinant, we demonstrate that the ground state in the gapless region exhibits a peculiar longitudinal spin-spin correlation. The entangled nature of the ground state is also disclosed by the evaluation of its entanglement entropy. At low temperature, new behavior of specific heat is predicted. We also propose an experimental protocol for observing the new phenomenon due to the ring frustration.

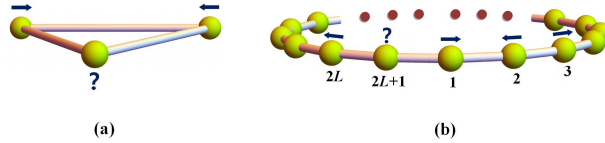
## 1. Introduction

Ising spin chain in a transverse field

$$H = J \sum_{j=1}^N \sigma_j^x \sigma_{j+1}^x - h \sum_{j=1}^N \sigma_j^z \quad (1)$$

with Pauli matrices  $\sigma_j^\alpha$  ( $\alpha = x, z$ ) is a well-known prototype for demonstrating quantum phase transition [1]. Jordan-Wigner transformation can be employed to solve it [2, 3, 4]. By neglecting the boundary effect in thermodynamic limit, Lieb *et al.* defined and solved a "c-cycle" problem. While the original problem without any approximation is called an "a-cycle" one [3, 5]. In the c-cycle problem, the thermodynamic limit is performed at the beginning, which brings the model to a free fermion problem. While in the a-cycle problem, if we consider a perfect periodic boundary condition (PBC) for the original spin model, we get a constraint fermion problem and have to keep an arbitray  $N$  during the calculation. We only have the opportunity to take the limit  $N \rightarrow \infty$  at the end of calculation.

The theoretical properties of the model (1) have been related to real materials since decades ago [5, 6]. Researchers have also been looking for nowadays state-of-art techniques, such as the ones based on laser-cooled and trapped atomic ions, to mimic this model [7, 8]. But these artificial systems can only produce finite lattices in principle, through which we hope to see the trend for large enough systems. The system with perfect PBC can be realized through a ring geometric optical lattices [9], which demands a thorough comprehension of the a-cycle problem. To the best of our knowledge, it has not been treated seriously up to now [3]. In this work, we shall develop a systematic method of band structure analysis to handle it and produce exact result that can match the full degrees of freedom of the spin model. The results will also be confirmed by an alternative method of exact diagonalization on small systems.



**Figure 1.** The main focus of this paper: transverse Ising ring with odd number of lattice sites: (a)  $N = 3$ , (b)  $N = 2L + 1$  ( $L = 1, 2, 3, \dots$ ). The Hamiltonian is shown in (1), which exhibits a ring frustration due to antiferromagnetic seam ( $J > 0$ ).

On the other hand, frustration is an intriguing topic. Very few frustrated models can be solved exactly [10]. To seek for nontrivial phenomenon, we mainly focus on the antiferromagnetic ( $J > 0$ ) system with PBC and large enough  $N \in \text{Odd}$ , because it suffers a *ring frustration* [11, 12] as a result of antiferromagnetic seam [13] (please see Fig. 1). Notice the ring frustration here is not a short range type of the usual case. One may ask whether the oddity of  $N$  plays a meaningful character in the a-cycle problem when  $N \rightarrow \infty$ . The answer is affirmative. By the rigorous solution, we demonstrate that the combination of the a-cycle problem and ring frustration does result in a dramatical consequence. To understand the fascinating result in a contrastive manner, we also discuss the system without any frustration, i.e. with  $N \in \text{Even}$ .

We arrange the contents of this paper as follows. In Section 2, we discuss the details about how the periodic spin problem is turned into a fermionic a-cycle one. In Section 3, we dwell on the a-cycle problem without ring frustration ( $N \in \text{Even}$ ). We develop the method of band structure analysis. In Section 4, we work on the a-cycle problem with ring frustration ( $N \in \text{Odd}$ ). We demonstrate that the presence of ring frustration will induce an interesting gapless spectrum above the ground state in the strong antiferromagnetic region. We demonstrate that the ground state exhibits a strong longitudinal spin-spin correlation and possesses a considerably large entropy of entanglement. We also give finite-temperature properties of the gapless region, including the density of states (DOS) and the specific heat. In Section 5, we propose an experimental protocol with special concern of the realization of ring frustration. At last, we give a discussion in Section 6.

## 2. Jordan-Wigner fermions and the statement of the a-cycle problem

It is convenient to convert the Pauli matrices to the raising and lowering operators,

$$\sigma_j^x = \sigma_j^+ + \sigma_j^-, \sigma_j^z = 2\sigma_j^+ \sigma_j^- - 1. \quad (2)$$

By introducing the Jordan-Wigner fermions that abide by the non-local relations,

$$\sigma_1^+ = c_1^\dagger, \quad \sigma_j^+ = c_j^\dagger \exp(i\pi \sum_{l<j} c_l^\dagger c_l), \quad (3)$$

the spin model, (1), can be transformed to

$$\begin{aligned} H = Nh - 2h \sum_{j=1}^N c_j^\dagger c_j + J \sum_{j=1}^{N-1} (c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1}) \\ - J \exp(i\pi M)(c_N^\dagger - c_N)(c_1^\dagger + c_1), \end{aligned} \quad (4)$$

where the total number of fermions,  $M = \sum_{j=1}^N c_j^\dagger c_j$ , does not conserve. But the parity of the system does, which is defined as

$$P = \exp(i\pi M) = (-1)^M. \quad (5)$$

The vacuum state, devoid of any fermions, corresponds to the full polarized spin state (spin down),

$$|0\rangle = |\downarrow\downarrow\downarrow \cdots \downarrow\rangle. \quad (6)$$

(4) defines the full a-cycle problem [3, 6].

As a comparison, the c-cycle problem is defined by neglecting the last term,  $-J[\exp(i\pi M) + 1](c_N^\dagger - c_N)(c_1^\dagger + c_1)$ , in [3]

$$\begin{aligned} H = Nh - 2h \sum_{j=1}^N c_j^\dagger c_j + J \sum_{j=1}^N (c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1}) \\ - J[\exp(i\pi M) + 1](c_N^\dagger - c_N)(c_1^\dagger + c_1). \end{aligned} \quad (7)$$

In doing so, one has accomplished the thermodynamic limit. Thus the c-cycle problem becomes a free fermion one [4].

While for a system with perfect ring geometry, there holds a precise condition on the spins,  $\sigma_{N+j}^\alpha = \sigma_j^\alpha$ . With no ends (or boundaries) existing, nothing in (4) could be neglected. We have to keep an arbitrary  $N$  in the calculation. We hope to get a result containing  $N$  as a variable thus it facilitates us to take the limit,  $N \rightarrow \infty$ .

Then, we can discern the different consequences of the limits,  $N(\in \text{Even}) \rightarrow \infty$  and  $N(\in \text{Odd}) \rightarrow \infty$ .

One should notice that, although there holds a PBC for the spin operators, a priori PBC should not be imposed on the fermions since an anti-PBC is also a reasonable choice. We will demonstrate both of them,  $c_{N+j} = c_j$  (PBC) and  $c_{N+j} = -c_j$  (anti-PBC), are indispensable to restore the full degrees of freedom of the original spin model, (1), exactly. We will see that the parity,  $P$ , will be fixed by the boundary condition of the fermions.

### 3. A-cycle problem without ring frustration ( $N \in \text{Even}$ )

Let us see the case without ring frustration first. To make the Fourier transformation

$$c_q = \frac{1}{\sqrt{N}} \sum_{j=1}^N c_j \exp(i q j) \quad (8)$$

available for solving the fermionic problem, we found the boundary condition must be bound up with the parity. So there are two routes to be followed. When  $M \in \text{odd}$ , we call it the *odd channel (o)* and when  $M \in \text{even}$ , the *even channel (e)* respectively. The procedure inevitably becomes a little tedious. In the following, we delicately use notations to make the deductions as clear as possible. For example, we use the notations  $N \in \text{Even}$  and  $M \in \text{even}$ , although *Even* and *even* are the same thing.

In fact, for the case of  $N \in \text{Even}$ , Schultz *et al.* [14] had discussed the contribution of the two channels in context of the classical two-dimensional Ising model in the same essence. But their discussion on the thermal states of the classical two-dimensional Ising model only corresponds to the ground state property of the quantum transverse Ising model. In this section, we discuss the quantum model directly and develop a method of band structure analysis for both ground states and excitations.

#### 3.1. Diagonalization in the odd channel

In the odd channel ( $M \in \text{odd}$ ), the Jordan-Wigner fermions must obey PBC:  $c_{N+j} = c_j$ , and the momentum in the first Brillouin zone (1st BZ) must take a value in the set

$$q^{(E,o)} = \left\{ -\frac{N-2}{N}\pi, \dots, -\frac{2}{N}\pi, 0, \frac{2}{N}\pi, \dots, \frac{N-2}{N}\pi, \pi \right\}, \quad (9)$$

where the superscript  $(E,o)$  denotes  $N \in \text{Even}$  ( $E$ ) and  $M \in \text{odd}$  ( $o$ ). After the Fourier transformation, the Hamiltonian can be diagonalized by the Bogoliubov transformation

$$\eta_q = u_q c_q - i v_q c_{-q}^\dagger \quad (10)$$

as

$$\begin{aligned} H^{(E,o)} = & (J-h) \left( 2c_0^\dagger c_0 - 1 \right) - (J+h) \left( 2c_\pi^\dagger c_\pi - 1 \right) \\ & + \sum_{q \in q^{(E,o)}, q \neq 0, \pi} \omega(q) \left( 2\eta_q^\dagger \eta_q - 1 \right), \end{aligned} \quad (11)$$

where

$$\begin{aligned} u_q^2 &= \frac{1}{2} \left( 1 + \frac{\epsilon(q)}{\omega(q)} \right), v_q^2 = \frac{1}{2} \left( 1 - \frac{\epsilon(q)}{\omega(q)} \right), 2u_q v_q = \frac{\Delta(q)}{\omega(q)}, \\ \omega(q) &= \sqrt{\epsilon(q)^2 + \Delta(q)^2}, \epsilon(q) = J \cos q - h, \Delta(q) = J \sin q. \end{aligned} \quad (12)$$

Notice there is no need of Bogoliubov transformation for  $q = 0$  and  $\pi$ .

### 3.2. Diagonalization in the even channel

In the even channel ( $M \in \text{even}$ ), the Jordan-Wigner fermions must obey anti-PBC:  $c_{N+j} = -c_j$ , and the momentum in the 1st BZ must take a value in the set

$$q^{(E,e)} = \left\{ -\frac{N-1}{N}\pi, \dots, -\frac{1}{N}\pi, \frac{1}{N}\pi, \dots, \frac{N-1}{N}\pi \right\}. \quad (13)$$

The diagonalized Hamiltonian is

$$H^{(E,e)} = \sum_{q \in q^{(E,e)}} \omega(q) (2\eta_q^\dagger \eta_q - 1). \quad (14)$$

### 3.3. Band structure of the energy levels

**3.3.1. The ground state(s) and energy gap** The lowest energy state in the odd channel is

$$|E_0^{(E,o)}\rangle = c_\pi^\dagger |\phi^{(E,o)}\rangle, \quad (15)$$

where  $|\phi^{(E,o)}\rangle$  is a pure BCS-like function,

$$|\phi^{(E,o)}\rangle = \prod_{q \in q^{(E,o)}, 0 < q < \pi} (u_q + iv_q c_q^\dagger c_{-q}^\dagger) |0\rangle, \quad (16)$$

where the vacuum state  $|0\rangle$  is (6). Its energy reads

$$E_0^{(E,o)} = |J - h| - (J - h) - \sum_{q \in q^{(E,o)}} \omega(q). \quad (17)$$

Notice that the fermionic BCS state  $|\phi^{(E,o)}\rangle$  itself can not be a valid state for the original spin model because of the parity constraint.

Likewise, The lowest energy state in the even channel reads

$$|E_0^{(E,e)}\rangle = |\phi^{(E,e)}\rangle, \quad (18)$$

where

$$|\phi^{(E,e)}\rangle = \prod_{q \in q^{(E,e)}, q > 0} (u_q + iv_q c_q^\dagger c_{-q}^\dagger) |0\rangle. \quad (19)$$

Its energy reads

$$E_0^{(E,e)} = - \sum_{q \in q^{(E,e)}} \omega(q) \quad (20)$$

If  $N$  is small, we always have  $E_0^{(E,e)} < E_0^{(E,o)}$ , so  $|E_0^{(E,e)}\rangle$  is the ground state.

If  $N \rightarrow \infty$ ,  $|E_0^{(E,e)}\rangle$  is still the ground state for  $J < h$  and there is a gap,  $\Delta_{gap} = 2(h - J)$ , to the first excited state  $|E_0^{(E,o)}\rangle$ . Above  $|E_0^{(E,o)}\rangle$ , there is a continuum band of excitations. While for  $J > h$ ,  $|E_0^{(E,e)}\rangle$  and  $|E_0^{(E,o)}\rangle$  become the degenerate ground states and there is a gap,  $\Delta_{gap} = 4(J - h)$ , above them. Now, the sum in the ground state energy, (20), can be replaced with an integral that can be worked out, so we get

$$\left. \frac{E_0^{(E,e)}}{N} \right|_{N \rightarrow \infty} \rightarrow \frac{-2|J - h|}{\pi} E \left( \frac{-4Jh}{(J - h)^2} \right), \quad (21)$$

where  $E(x)$  is the complete elliptic integral of the second kind. (21) is non-analytic at  $J/h = 1$ , because its second derivative in respect of  $J/h$  has a logarithmic divergent peak  $\sim (1/\pi) \ln |J/h - 1|$ . So in fact, we have a critical point at  $J = h$ . These conclusions are the same as the ones in previous investigations [15].

We have checked that the two states, (15) and (18), in the limit  $h \rightarrow 0$  correspond to two GHZ spin states in  $\sigma^x$  representation,

$$\lim_{h \rightarrow 0} |E_0^{(E,e)}\rangle = \frac{1}{\sqrt{2}}(|\cdots \leftarrow_{j-1}, \rightarrow_j, \leftarrow_{j+1}, \rightarrow_{j+2}, \cdots\rangle - |\cdots \rightarrow_{j-1}, \leftarrow_j, \rightarrow_{j+1}, \leftarrow_{j+2}, \cdots\rangle), \quad (22)$$

$$\lim_{h \rightarrow 0} |E_0^{(E,o)}\rangle = \frac{1}{\sqrt{2}}(|\cdots \leftarrow_{j-1}, \rightarrow_j, \leftarrow_{j+1}, \rightarrow_{j+2}, \cdots\rangle + |\cdots \rightarrow_{j-1}, \leftarrow_j, \rightarrow_{j+1}, \leftarrow_{j+2}, \cdots\rangle), \quad (23)$$

respectively.

**3.3.2. Analysis of bands** The degrees of freedom (DOF) of the fermionic problem are  $2^N$  for both channels, so we get  $2^{N+1}$  DOF totally, which is redundantly twice of the DOF of the original spin model. However, the odd channel requires an odd parity and the even channel an even parity. This parity constraint helps us to obliterate the redundant DOF in each channel exactly and reconstruct the band structure of the original spin problem.

We can construct all excited energy levels by the BCS functions (19) and (16) precisely. All energy levels can be grouped into bands that are labelled by a set of indexes  $(P, Q^{(E)}, n_0, n_\pi)$ , where  $P$  is the parity defined in (5),  $Q^{(E)}$  is a quasi-particle number defined as

$$Q^{(E)} = \sum_{q \in q^{(E,o)} \cup q^{(E,e)}} n_q, \quad (24)$$

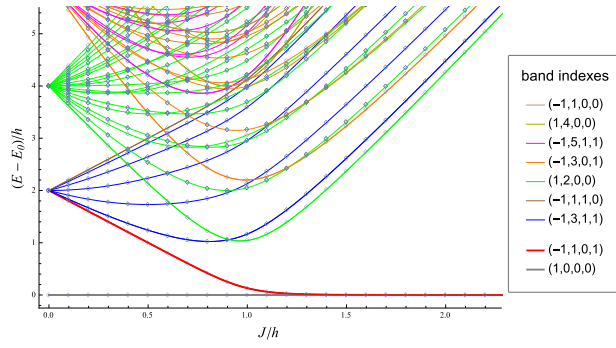
$n_0 = c_0^\dagger c_0$ , and  $n_\pi = c_\pi^\dagger c_\pi$ . For example, the band indexes of the two states discussed above are  $(1, 0, 0, 0)$  and  $(-1, 1, 0, 1)$  for  $|E_0^{(E,e)}\rangle$  and  $|E_0^{(E,o)}\rangle$  respectively. These two bands contains only one level each. From all bands of the fermionic problem, we can pick out the valid ones for the spin model according to the parity constraint. Several valid bands of low energy states are listed in Table 1. The energy value of each state is readily read out from the diagonalized Hamiltonian, (11) and (14). The band structure is available for arbitrary  $N$  ( $N \in \text{Even}$ ,  $2 \leq N < \infty$ ). It is noteworthy that the invalid bands, for example such as  $(1, 1, 0, 0)$  and  $(-1, 2, 0, 1)$ , are prohibited by the parity constraint of each channel.

To testify the band structure further, we compare it with the result by an exact diagonalization of the transverse Ising model with a small size, say  $N = 12$ . The comparison is shown in Fig. 2, where a perfect coincidence can be clearly seen. So we see our method can restore the full degrees of freedom of the spin model.

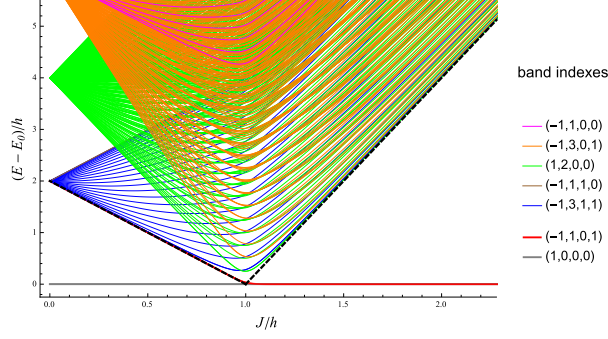
The band structure for a larger system, say  $N = 50$ , is exemplified in Fig. 3, through which we can see the trend for a large enough system,  $N \rightarrow \infty$ . At the critical point, the bottom levels of many bands satisfying  $P = 1$  or  $P \times n_\pi = -1$  will touch the critical point, which will result in a divergent DOS.

Valid Bands ( $P, Q^{(E)}, \eta_0, \eta_\pi$ )	Fermionic states ( $q \neq 0, \pi$ )	Number of states
odd channel ( $M \in odd$ )		
$(-1, 1, 0, 1)$	$c_\pi^\dagger  \phi^{(E,o)}\rangle =  E_0^{(E,o)}\rangle$	1
$(-1, 1, 1, 0)$	$c_0^\dagger  \phi^{(E,o)}\rangle$	1
$(-1, 1, 0, 0)$	$\eta_q^\dagger  \phi^{(E,o)}\rangle$	$C_{N-2}^1$
$(-1, 3, 0, 0)$	$\eta_{q_1}^\dagger \eta_{q_2}^\dagger \eta_{q_3}^\dagger  \phi^{(E,o)}\rangle$	$C_{N-2}^3$
$(-1, 3, 0, 1)$	$\eta_{q_1}^\dagger \eta_{q_2}^\dagger c_\pi^\dagger  \phi^{(E,o)}\rangle$	$C_{N-2}^2$
$(-1, 3, 1, 0)$	$\eta_{q_1}^\dagger \eta_{q_2}^\dagger c_0^\dagger  \phi^{(E,o)}\rangle$	$C_{N-2}^2$
$(-1, 3, 1, 1)$	$\eta_{q_1}^\dagger c_0^\dagger c_\pi^\dagger  \phi^{(E,o)}\rangle$	$C_{N-2}^1$
$\vdots$	$\vdots$	$\vdots$
even channel ( $M \in even$ )		
$(1, 0, 0, 0)$	$ \phi^{(E,e)}\rangle =  E_0^{(E,e)}\rangle$	1
$(1, 2, 0, 0)$	$\eta_{q_1}^\dagger \eta_{q_2}^\dagger  \phi^{(E,e)}\rangle$	$C_N^2$
$(1, 4, 0, 0)$	$\eta_{q_1}^\dagger \eta_{q_2}^\dagger \eta_{q_3}^\dagger \eta_{q_4}^\dagger  \phi^{(E,e)}\rangle$	$C_N^4$
$\vdots$	$\vdots$	$\vdots$

**Table 1.** The valid bands satisfying the odd or even parity constraint for the case  $N \in Even$ . Invalid bands are not included. The energy value of each state is readily read out from the diagonalized Hamiltonian, (11) or (14).



**Figure 2.** The band structure of low-energy levels for a system of  $N = 12$ . The purpose of this figure is to check the band structure for  $N \in Even$  disclosed in the text. The dingbat diamonds (") denote the results from exact diagonalization on the original spin model, which are in perfect coincidence with the bands of levels. The true ground state, (18), with band indexes (1,0,0,0) is set as a reference.



**Figure 3.** The band structure of low-energy levels for a system of  $N = 50$ . From this figure, one can figure out the trend for  $N \rightarrow \infty$  (we still hold  $N \in \text{Even}$ ). The dashed black line is the lower bound of excitations when  $N \rightarrow \infty$ , whose intersecting point at  $J/h = 1$  is a critical point as disclosed by (20). The bottom levels of many bands will touch this critical point, which results in a divergent DOS. At both sides of the critical point, the system is gapped. Not all bands above the dashed black line are shown.

#### 4. A-cycle problem with ring frustration ( $N \in \text{Odd}$ )

Now we turn to the interesting case with frustration (Fig. 1). The procedure is almost the same. But the story is totally different. In the strong antiferromagnetic region, we find a gapless spectrum above the ground state if the system is large enough.

##### 4.1. Diagonalization in the odd channel

In the odd channel ( $M \in \text{odd}$ ), the Jordan-Wigner fermions must obey PBC:  $c_{N+j} = c_j$ , and the momentum in the 1st BZ must take a value in the set

$$q^{(O,o)} = \left\{ -\frac{N-1}{N}\pi, \dots, -\frac{2}{N}\pi, 0, \frac{2}{N}\pi, \dots, \frac{N-1}{N}\pi \right\}. \quad (25)$$

The diagonalized Hamiltonian is

$$H^{(O,o)} = (J - h) \left( 2c_0^\dagger c_0 - 1 \right) + \sum_{q \in q^{(O,o)}, q \neq 0} \omega(q) \left( 2\eta_q^\dagger \eta_q - 1 \right). \quad (26)$$

##### 4.2. Diagonalization in the even channel

In the even channel ( $M \in \text{even}$ ), the Jordan-Wigner fermions must obey anti-PBC:  $c_{N+j} = -c_j$ , and the momentum in the 1st BZ must take a value in the set

$$q^{(O,e)} = \left\{ -\frac{N-2}{N}\pi, \dots, -\frac{1}{N}\pi, \frac{1}{N}\pi, \dots, \frac{N-2}{N}\pi, \pi \right\}. \quad (27)$$

The diagonalized Hamiltonian is

$$H^{(O,e)} = -(J + h) \left( 2c_\pi^\dagger c_\pi - 1 \right) + \sum_{q \in q^{(O,e)}, q \neq \pi} \omega(q) \left( 2\eta_q^\dagger \eta_q - 1 \right). \quad (28)$$



## 4.3. Band structure of the energy levels

4.3.1. *The ground state* The lowest energy state in the odd channel reads

$$|E_0^{(O,o)}\rangle = c_0^\dagger |\phi^{(O,o)}\rangle, \quad (29)$$

where

$$|\phi^{(O,o)}\rangle = \prod_{q \in q^{(O,o)}, q > 0} \left( u_q + i v_q c_q^\dagger c_{-q}^\dagger \right) |0\rangle. \quad (30)$$

Its energy reads

$$E_0^{(O,o)} = |J - h| + (J - h) - \sum_{q \in q^{(O,o)}} \omega(q). \quad (31)$$

The lowest energy state in the even channel reads

$$|E_0^{(O,e)}\rangle = \eta_{\frac{\pi}{N}}^\dagger c_\pi^\dagger |\phi^{(O,e)}\rangle, \quad (32)$$

where

$$|\phi^{(O,e)}\rangle = \prod_{q \in q^{(O,e)}, 0 < q < \pi} \left( u_q + i v_q c_q^\dagger c_{-q}^\dagger \right) |0\rangle. \quad (33)$$

Its energy reads

$$E_0^{(O,e)} = 2\omega\left(\frac{\pi}{N}\right) - \sum_{q \in q^{(O,e)}} \omega(q). \quad (34)$$

If  $N$  is small, we always have  $E_0^{(O,o)} < E_0^{(O,e)}$ , so  $|E_0^{(O,o)}\rangle$  is the ground state and  $|E_0^{(O,e)}\rangle$  is the first excited state.

If  $N \rightarrow \infty$ , the state  $|E_0^{(O,o)}\rangle$  (29) is the ground state. In the region  $J < h$ , there is a gap,  $\Delta_{\text{gap}} = 2(h - J)$ , to the first excited state  $|E_0^{(O,e)}\rangle$  (32). In the region  $J > h$ , the energy gap between  $|E_0^{(O,o)}\rangle$  and  $|E_0^{(O,e)}\rangle$  disappears. But we notice that there is no energy gap between  $|E_0^{(O,e)}\rangle$  and the next excitation, and so forth. In fact there appears a gapless spectrum above the ground state  $|E_0^{(O,o)}\rangle$ . We will discuss this gapless spectrum later in detail in Section 4.3.3. While at  $J = h$ , the ground state energy,

$$\left. \frac{E_0^{(O,o)}}{N} \right|_{N \rightarrow \infty} \rightarrow \frac{-2|J - h|}{\pi} E\left(\frac{-4Jh}{(J - h)^2}\right) + \frac{2}{N}(J - h)\theta(J - h), \quad (35)$$

with a Heaviside step function  $\theta(x)$  is still non-analytic. In fact, the self-duality still holds for the frustrated ring system with odd  $N$  and ensures the occurring of quantum phase transition at  $J = h$ . One can see this clear by defining new Ising-type operators,

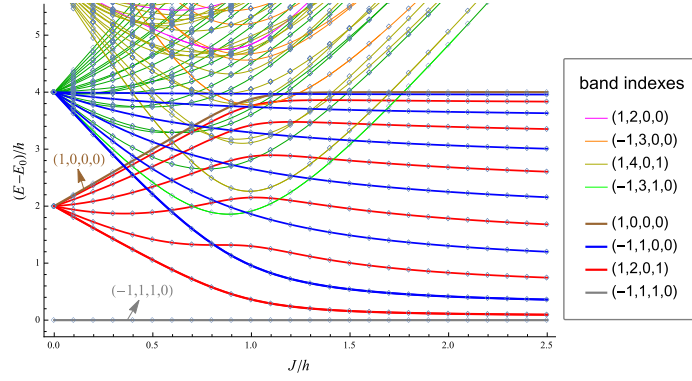
$$\tau_j^z = -\sigma_j^x \sigma_{j+1}^x, \tau_j^x = (-1)^j \prod_{l < j} \sigma_l^z, \quad (36)$$

to get a dual form of Hamiltonian [16]

$$H = -J \sum_{j=1}^N \tau_j^z + h \sum_{j=1}^N \tau_j^x \tau_{j+1}^x. \quad (37)$$

Valid Bands ( $P, Q^{(O)}, \eta_0, \eta_\pi$ )	Fermionic state ( $q \neq 0, \pi$ )	Number of states
odd channel ( $M \in \text{odd}$ )		
$(-1, 1, 0, 0)$	$\eta_q^\dagger  \phi^{(O,o)}\rangle$	$C_{N-1}^1$
$(-1, 1, 1, 0)$	$c_0^\dagger  \phi^{(O,o)}\rangle =  E_0^{(O,o)}\rangle$	1
$(-1, 3, 0, 0)$	$\eta_{q_1}^\dagger \eta_{q_2}^\dagger \eta_{q_3}^\dagger  \phi^{(O,o)}\rangle$	$C_{N-1}^3$
$(-1, 3, 1, 0)$	$\eta_{q_1}^\dagger \eta_{q_2}^\dagger c_0^\dagger  \phi^{(O,o)}\rangle$	$C_{N-1}^2$
$\vdots$	$\vdots$	$\vdots$
even channel ( $M \in \text{even}$ )		
$(1, 0, 0, 0)$	$ \phi^{(O,e)}\rangle$	1
$(1, 2, 0, 0)$	$\eta_{q_1}^\dagger \eta_{q_2}^\dagger  \phi^{(O,e)}\rangle$	$C_{N-1}^2$
$(1, 2, 0, 1)$	$\eta_q^\dagger c_\pi^\dagger  \phi^{(O,e)}\rangle$	$C_{N-1}^1$
$\vdots$	$\vdots$	$\vdots$

**Table 2.** The valid bands satisfying the odd or even parity constraint for the case  $N \in \text{Odd}$ . The energy value of each state is readily read out from the diagonalized Hamiltonian, (26) or (28).

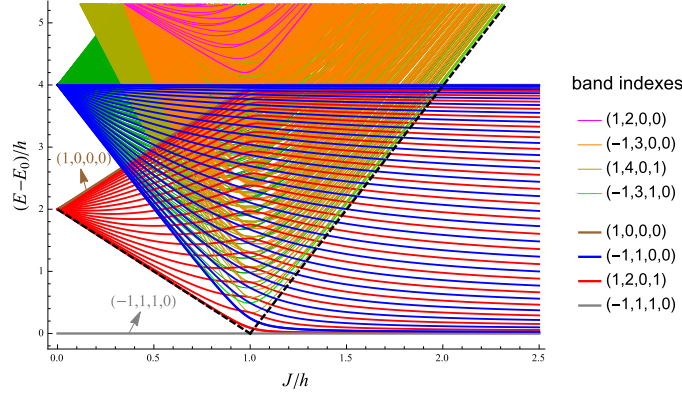


**Figure 4.** The band structure of low-energy levels for a system of  $N = 13$ . The purpose of this figure is to check the band structure for  $N \in \text{Odd}$  disclosed in the text. The bands of levels are in perfect coincidence with the results from exact diagonalization on the original spin model (shown as dingbat diamonds "◊"). The true ground state, (29), with band indexes  $(-1, 1, 1, 0)$  is set as a reference.

4.3.2. *Analysis of bands* By defining the quasi-particle number

$$Q^{(O)} = \sum_{q \in q^{(O,o)} \cup q^{(O,e)}} n_q, \quad (38)$$

we can use the set of indexes  $(P, Q^{(O)}, n_0, n_\pi)$  to label all the fermionic bands as we have done in Section 3.3.2. From the fermionic bands in each channel, we can pick out the valid ones for the original spin model according to the parity constraint. The valid bands of several low energy levels are listed in Table 2. The energy value of each state is readily read out from the diagonalized Hamiltonian, (26) or (28). The band structure is available for arbitrary  $N$  ( $N \in \text{Odd}$ ,  $3 \leq N < \infty$ ).



**Figure 5.** The band structure of low-energy levels for a system of  $N = 51$ . From this figure, one can figure out the trend for  $N \rightarrow \infty$  ( $N \in \text{Odd}$  is still hold). In contrast with the case of  $N \in \text{Even}$  in Fig. 3, the low excitations is dramatically changed in the region  $J/h > 1$  due to the presence of ring frustration. If  $N \rightarrow \infty$ , we can still draw a dashed black line, whose intersecting point at  $J/h = 1$  is a critical point as disclosed by (35). And the bottom levels of many bands satisfying  $P = -1$  or  $P \times n_\pi = 1$  will touch this critical point, which results in a divergent DOS. There is an energy gap for the region  $J/h < 1$ . However, the excitations for the region  $J/h > 1$  are gapless, where the energy interval of width  $4h$  is depleted by  $N + 1$  levels occupied by  $2N$  states involving 4 bands:  $(-1, 1, 1, 0)$ ,  $(1, 2, 0, 1)$ ,  $(-1, 1, 0, 0)$ , and  $(1, 0, 0, 0)$ . Not all bands above the dashed black line are shown.

In Fig. 4, we testify the band structure further by comparing it with the result by the exact diagonalization on a system of  $N = 13$ . Perfect coincidence is observed. So we see our method restores the full degrees of freedom of the spin model.

In Fig. 5, the band structure for a larger system with  $N = 51$  is exemplified, through which we can see the trend for a large enough system,  $N \rightarrow \infty$ . At the critical point, the bottom levels of many bands satisfying  $P = -1$  or  $P \times n_\pi = 1$  will touch the critical point, which will result in a divergent DOS.

**4.3.3. Gapless spectrum in the region  $J > h$**  In the strong antiferromagnetic region  $J > h$ , there forms a gapless spectrum when  $N \rightarrow \infty$ . It contains  $2N$  states involving 4 interwoven bands. They occupy  $N + 1$  energy levels. The ground state  $|E_0^{(O,o)}\rangle$  with band indexes  $(-1, 1, 1, 0)$  lies at the bottom. We relabel it as

$$|E_0\rangle = |E_0^{(O,o)}\rangle = c_0^\dagger |\phi^{(O,o)}\rangle. \quad (39)$$

The upper-most state is  $|\phi^{(O,e)}\rangle$  with indexes  $(1, 0, 0, 0)$ . We relabel it as

$$|E_\pi\rangle = |\phi^{(O,e)}\rangle. \quad (40)$$

The other two bands are:

$$|E_q\rangle = \eta_q^\dagger c_\pi^\dagger |\phi^{(O,e)}\rangle, (q \in q^{(O,e)}, q \neq \pi) \quad (41)$$

with indexes  $(1, 2, 0, 1)$  and

$$|E_q\rangle = \eta_q^\dagger |\phi^{(O,o)}\rangle, (q \in q^{(O,o)}, q \neq 0) \quad (42)$$

with indexes  $(-1, 1, 0, 0)$ . If  $N$  is finite,  $|E_0\rangle$  and  $|E_\pi\rangle$  are nondegenerate, while other  $|E_q\rangle$ 's are doubly degenerate. When  $N \rightarrow \infty$ , these  $2N$  states deplete the energy interval of width

$$\Delta_w = E_\pi - E_0 \xrightarrow{N \rightarrow \infty} 4h \quad (43)$$

between  $|E_0\rangle$  and  $|E_\pi\rangle$ . This result is beyond the familiar schematic picture for quantum phase transition [15].

*Perturbative theory* To understand the formation of gapless spectrum, let us see a perturbative picture in the strong antiferromagnetic region  $J > h$ . The first term of (1)

$$H_0 = J \sum_{j=1}^N \sigma_j^x \sigma_{j+1}^x \quad (44)$$

is a classical Ising model, whose ground states are highly degenerate as an effect of antiferromagnetic seam [13]. By choosing the representation of  $\sigma_j^z$ , i.e.  $\sigma_j^z |\uparrow_j\rangle = |\uparrow_j\rangle$  and  $\sigma_j^z |\downarrow_j\rangle = -|\downarrow_j\rangle$ , and denoting the two eigenstates of  $\sigma_j^x$  as  $|\rightarrow_j\rangle = (|\uparrow_j\rangle + |\downarrow_j\rangle)/\sqrt{2}$  and  $|\leftarrow_j\rangle = (|\uparrow_j\rangle - |\downarrow_j\rangle)/\sqrt{2}$  [1], we can express its  $2N$ -fold degenerate ground states as kink states [11]:

$$\begin{aligned} |K(j), \rightarrow\rangle &= |\cdots, \leftarrow_{j-1}, \rightarrow_j, \rightarrow_{j+1}, \leftarrow_{j+2}, \cdots\rangle \\ |K(j), \leftarrow\rangle &= |\cdots, \rightarrow_{j-1}, \leftarrow_j, \leftarrow_{j+1}, \rightarrow_{j+2}, \cdots\rangle. \end{aligned} \quad (45)$$

where kinks occur between sites  $j$  and  $j+1$ . The classical Ising system falls into one of these states by spontaneous symmetry breaking [10]. But they are not eigenstates of the full quantum system. The second term of (1),

$$V = -h \sum_{j=1}^N \sigma_j^z, \quad (46)$$

as a source of quantum fluctuation, plays the role of perturbation when  $h/J$  is small. We relabel the kink states as

$$\begin{aligned} |2j-1\rangle &= |K(j), \rightarrow\rangle \\ |2j\rangle &= |K(j), \leftarrow\rangle. \end{aligned} \quad (47)$$

Then by the simplest perturbative scheme based on these levels, we can deduce the matrix form of the full spin Hamiltonian  $H = H_0 + V$  ( $2N \times 2N$ ), whose diagonal elements read

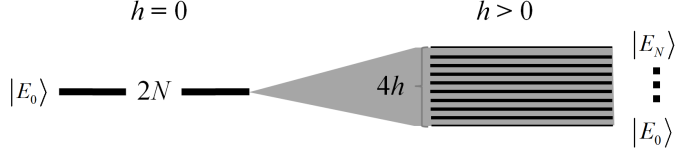
$$H_{2j-1, 2j-1} = H_{2j, 2j} = J \quad (48)$$

and off-diagonal elements read

$$H_{2j, 2j+1} = H_{2j-1, 2j+2} = H_{2j+1, 2j} = H_{2j+2, 2j-1} = -h. \quad (49)$$

Other elements are zero. We can arrive at an effective Hamiltonian approximately,

$$\begin{aligned} H \approx H_{\text{eff}} &= J \sum_{j=1}^N (|2j-1\rangle \langle 2j-1| + |2j\rangle \langle 2j|) \\ &\quad - h \sum_{j=1}^N (|2j\rangle \langle 2j+1| + |2j-1\rangle \langle 2j+2| + \text{h.c.}). \end{aligned} \quad (50)$$



**Figure 6.** Schematic diagram of the formation of gapless spectrum above the ground state from a perturbative point of view.

Now by introducing a Fourier transformation

$$|2j-1\rangle = \frac{1}{\sqrt{N}} \sum_k |a_k\rangle e^{ikj}, |2j\rangle = \frac{1}{\sqrt{N}} \sum_k |b_k\rangle e^{ikj} \quad (51)$$

with

$$k = -\frac{N-1}{N}\pi, \dots, -\frac{2}{N}\pi, 0, \frac{2}{N}\pi, \dots, \frac{N-1}{N}\pi, \quad (52)$$

we get

$$H_{\text{eff}} = \sum_k [J(|a_k\rangle \langle a_k| + |b_k\rangle \langle b_k|) - 2h(\cos k|b_k\rangle \langle a_k| + \cos k|a_k\rangle \langle b_k|)]. \quad (53)$$

We can diagonalize it as

$$H_{\text{eff}} = \sum_k [(J - 2h \cos k) |A_k\rangle \langle A_k| + (J + 2h \cos k) |B_k\rangle \langle B_k|] \quad (54)$$

by denoting

$$|A_k\rangle = \frac{1}{\sqrt{2}} (|a_k\rangle + |b_k\rangle), |B_k\rangle = \frac{1}{\sqrt{2}} (-|a_k\rangle + |b_k\rangle). \quad (55)$$

Thus the degenerate ground states of  $H_0$  is dispersed by  $V$  and form a band of  $N+1$  levels, i.e. the degeneracy is partly lifted. It is easy to check that the states  $|A_k\rangle$  have odd parity and the states  $|B_k\rangle$  have even parity. If  $N \rightarrow \infty$ , they form a gapless spectrum of width  $4h$ . They are good approximations of the lowest  $2N$  rigorous energy states. For example, the ground state of the system is

$$|A_0\rangle = \frac{1}{\sqrt{2N}} \sum_{j,\tau} |K(j), \tau\rangle \quad (56)$$

approximately. It is highly entangled. The excited eigenstates are recombinations of the  $2N$  kink states likewise. If  $N \rightarrow \infty$ , the low-lying excitations form a gapless spectrum of width  $4h$  as the schematic plot in Fig. 6.

As a relevant issue, we found that, if one deduces an effective two-dimensional classical Ising model for the quantum Ising chain by the first-order Suzuki-Trotter decomposition in the usual way [5, 17], the model will fail to capture the lifting of degeneracy of the kink states.

## 4.4. Correlation function of the ground state

Now we concern the longitudinal correlation function of the ground state. We still follow the strategy: try to work out the correlation function as a function of  $N \in \text{Odd}$ , then set the limit,  $N \rightarrow \infty$ , to see if there is any surprising result. For the gapless region, we find a new type of Toeplitz determinant that needs to be evaluated rigorously.

The two-point longitudinal spin-spin correlation function of the ground state is defined as

$$C_{r,N}^{xx} = \langle \phi^{(O,o)} | c_0 \sigma_j^x \sigma_{j+r}^x c_0^\dagger | \phi^{(O,o)} \rangle. \quad (57)$$

By introducing the operators,  $A_j = c_j^\dagger + c_j$  and  $B_j = c_j^\dagger - c_j$ , with the relations,  $A_j^2 = 1$  and  $A_j B_j = \exp(-i\pi c_j^\dagger c_j)$ , we get

$$C_{r,N}^{xx} = \langle \phi^{(O,o)} | c_0 B_j A_{j+1} B_{j+1} \dots B_{j+r-1} A_{j+r} c_0^\dagger | \phi^{(O,o)} \rangle. \quad (58)$$

By making use of the Wick's theorem and the contractions in respect of  $|\phi^{(O,o)}\rangle$ :  $\langle c_0 c_0^\dagger \rangle = 1$ ,  $\langle A_j c_0^\dagger \rangle = -\langle B_j c_0^\dagger \rangle = \frac{1}{\sqrt{N}}$ ,  $\langle A_j A_{j+r} \rangle = -\langle B_j B_{j+r} \rangle = \delta_{r,0}$ , and  $\langle B_j A_{j+r} \rangle = \mathcal{D}_{r+1}$  with

$$\mathcal{D}_r = \frac{1}{N} \sum_{q \in q^{(O,o)}, q \neq 0} \exp(-iqr) D(e^{iq}) - \frac{1}{N} \quad (59)$$

where

$$D(e^{iq}) = -\frac{J - h e^{iq}}{\sqrt{(J - h e^{iq})(J - h e^{-iq})}}. \quad (60)$$

We arrive at a Toeplitz determinant

$$C_{r,N}^{xx} = \begin{vmatrix} \mathcal{D}_0 + \frac{2}{N} & \mathcal{D}_{-1} + \frac{2}{N} & \cdots & \mathcal{D}_{-r+1} + \frac{2}{N} \\ \mathcal{D}_1 + \frac{2}{N} & \mathcal{D}_0 + \frac{2}{N} & \cdots & \mathcal{D}_{-r+2} + \frac{2}{N} \\ \dots & \dots & \dots & \dots \\ \mathcal{D}_{r-1} + \frac{2}{N} & \mathcal{D}_{r-2} + \frac{2}{N} & \cdots & \mathcal{D}_0 + \frac{2}{N} \end{vmatrix}. \quad (61)$$

It can be evaluated for arbitrary  $r$  and  $N$  directly. Notice that  $C_{r,N}^{xx} = C_{N-r,N}^{xx}$  due to the ring geometry. Next, we define

$$D_r = \frac{1}{N} \sum_{q \in q^{(O,o)}} \exp(-iqr) D(e^{iq}) \quad (62)$$

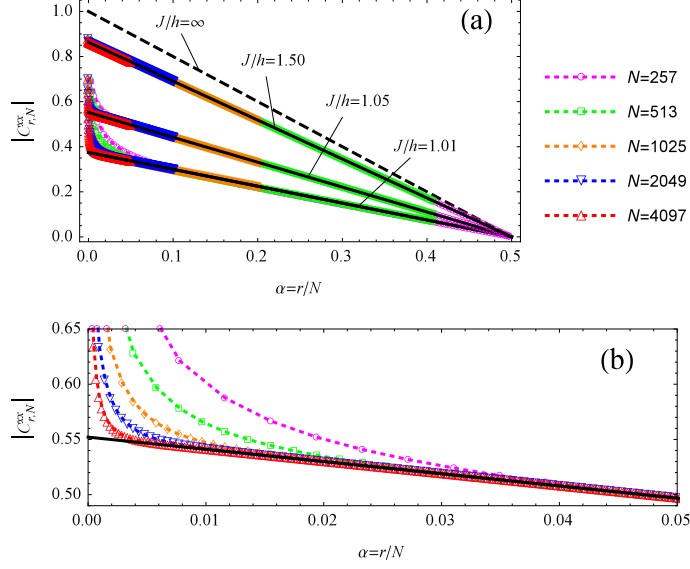
with appropriate predefined  $D(e^{i0})$ . Thus we have

$$\mathcal{D}_r = D_r - \frac{D(e^{i0})}{N} - \frac{1}{N} \quad (63)$$

In the gapped region ( $J < h$ ), we have  $D(e^{i0}) = 1$  and  $\mathcal{D}_r = D_r - \frac{2}{N}$ . The correlation function is given by

$$C_{r,N}^{xx} = \begin{vmatrix} D_0 & D_{-1} & \cdots & D_{-r+1} \\ D_1 & D_0 & \cdots & D_{-r+2} \\ \dots & \dots & \dots & \dots \\ D_{r-1} & D_{r-2} & \cdots & D_0 \end{vmatrix}. \quad (64)$$

This is the conventional Toeplitz determinant that has been investigated in the previous works [13], the correlation function decays exponentially with a finite correlation length  $\xi = -1/\ln(J/h)$ .



**Figure 7.** Longitudinal correlation functions for several selected values of  $J/h$  in the gapless region. The dashed black line in (a) is an exact result, (66), for  $J/h = \infty$  (i.e.  $h = 0$ ). In both (a) and (b), the colored dingbat data are direct rigorous evaluations of (61), while the black straight lines show the asymptotic behavior described by (73). (b) is a zoom-in plot for the case  $J/h = 1.05$ .

While in our focused gapless region ( $J/h > 1$ ), we have  $D(e^{i0}) = -1$  and  $\mathcal{D}_r = D_r$ . Then the correlation function is given by

$$C_{r,N}^{xx} = \Theta(r, N) = \begin{vmatrix} D_0 + \frac{2}{N} & D_{-1} + \frac{2}{N} & \cdots & D_{-r+1} + \frac{2}{N} \\ D_1 + \frac{2}{N} & D_0 + \frac{2}{N} & \cdots & D_{-r+2} + \frac{2}{N} \\ \cdots & \cdots & \cdots & \cdots \\ D_{r-1} + \frac{2}{N} & D_{r-2} + \frac{2}{N} & \cdots & D_0 + \frac{2}{N} \end{vmatrix} \quad (65)$$

The extra term  $\frac{2}{N}$  in each element makes it a totally new Toeplitz determinant. If one erases the term  $\frac{2}{N}$  when taking the limit  $N \rightarrow \infty$ , the conventional Toeplitz determinant is arrived. But we will show its non-local information is omitted in doing so. To this purpose, we retain the term  $\frac{2}{N}$  and keep  $N$  as a variable. Another reason for retaining the term  $\frac{2}{N}$  is the fact that the dimension of the determinant is  $r \times r$ , which can lead to a total contribution proportional to  $\frac{r}{N}$ .

First, let us see an exact result in the case  $h = 0$ . By (62), we have  $D_r = -\delta_{r,0}$ . Then (65) is reduced to

$$C_{r,N}^{xx} = (-1)^r (1 - 2\alpha), \quad (66)$$

where  $\alpha = \frac{r}{N}$ . If one takes the limit  $N \rightarrow \infty$  first and gets  $C_{r,N}^{xx} \approx (-1)^r$ , one would think this is a simple antiferromagnets. But if we take a value of  $\alpha \in (0, 1/2)$ , we see the exact result, (66), measures a non-local correlation because  $r = \alpha N \rightarrow \infty$ . Please notice that the ground state, (56), is an exact superposition of kink states, whose correlation function is exactly given by (66). This is purely a theoretical consequence of the model. The exact result is shown as the dashed black line in Fig. 7(a).

Second, we work out the asymptotic behaviour for arbitrary  $J > h$ . For a large enough system, we can substitute the sum in (62) with an integral to get

$$D_r \xrightarrow{N \rightarrow \infty} \int_{-\pi}^{\pi} \frac{dq}{2\pi} \exp(-iqr) D(e^{iq}). \quad (67)$$

Now we need to evaluate the new type of Toeplitz determinant in Eq. (65). Following the earlier procedure by McCoy and Wu [18, 19, 13], we have proved a theorem for this special case in Appendix A:

*Theorem: Consider a Toeplitz determinant  $\Theta(r, N)$  in (65) with*

$$D_n = \int_{-\pi}^{\pi} \frac{dq}{2\pi} D(e^{iq}) e^{-iqn}. \quad (68)$$

*If the generating function  $D(e^{iq})$  and  $\ln D(e^{iq})$  are continuous on the unit circle  $|e^{iq}| = 1$ , then the behavior for large  $N$  and  $r$  of  $\Theta(r, N)$  is given by*

$$\Theta(r, N) = \Delta_r \left(1 + \frac{2\alpha}{D(e^{i0})}\right), \quad (69)$$

where

$$\Delta_r = \mu^r \exp\left(\sum_{n=1}^{\infty} n d_{-n} d_n\right), \quad (70)$$

$$\mu = \exp\left[\int_{-\pi}^{\pi} \frac{dq}{2\pi} \ln D(e^{iq})\right], \quad (71)$$

$$d_n = \int_{-\pi}^{\pi} \frac{dq}{2\pi} e^{-iqn} \ln D(e^{iq}), \quad (72)$$

if the sum  $\sum_{n=1}^{\infty} n d_{-n} d_n$  is convergent.

By applying the above theorem to the gapless region ( $J > h$ ), we get an asymptotic behavior

$$C_{r,N}^{xx} = (-1)^r \left(1 - \frac{h^2}{J^2}\right)^{1/4} (1 - 2\alpha). \quad (73)$$

It is clear (73) coincides with (66). This asymptotic behavior is depicted in Fig. 7, which is perfectly coincident with the direct evaluations of (61). This surprising result is totally different from the conventional findings [1].

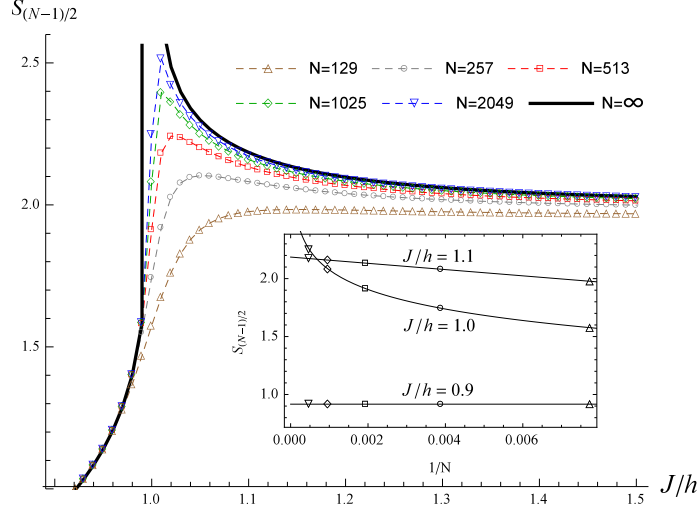
#### 4.5. Entanglement entropy of the ground state

Entanglement entropy is another powerful quantity for exhibiting the entangled nature of a system. We define the reduced density matrix  $\rho_l = \text{tr}_{N-l} |E_0^{(O,o)}\rangle \langle E_0^{(O,o)}|$  and the entanglement entropy (EE)  $S_l = -\text{tr}(\rho_l \log_2 \rho_l)$ , where the trace is performed on the spin states of contiguous sites from  $j=1$  to  $N-l$ . We can evaluate the EE numerically by utilizing the matrix [20, 21, 22]

$$\Gamma_l = \begin{vmatrix} \Pi_0 & \Pi_1 & \cdots & \Pi_{l-1} \\ \Pi_{-1} & \Pi_0 & \cdots & \Pi_{l-2} \\ \cdots & \cdots & \cdots & \cdots \\ \Pi_{1-l} & \Pi_{2-l} & \cdots & \Pi_0 \end{vmatrix} \text{ with } \Pi_l = \begin{vmatrix} 0 & -g_l \\ g_{-l} & 0 \end{vmatrix}, \quad (74)$$

where  $g_l = \mathcal{D}_{l-1} + \frac{2}{N}$ . Let  $V \in SO(2l)$  denote an orthogonal matrix that brings  $\Gamma_l$  into a block diagonal form such that  $\Gamma_l^C = V \Gamma_l V^T = \bigoplus_{m=0}^{l-1} (iv_m \sigma_y)$  with  $v_m \geq 0$ . Then  $S_l$





**Figure 8.** (Color online) Entanglement entropy  $S_{(N-1)/2}$  as a function of  $J/h$  for a sequence of number of lattice sites  $N$ . The inset shows examples of finite size scaling for extrapolating to  $N \rightarrow \infty$ . At the critical point, the numerical data fit a divergent behavior,  $S_{(N-1)/2} \sim \frac{1}{6} \log_2 N$ , coincident with the prediction by CFT [23].

is given by  $S_l = \sum_{m=0}^{l-1} H_2(\frac{1+v_m}{2})$  with  $H_2(x) = -x \log_2 x - (1-x) \log_2 (1-x)$ . The numerical results for  $l=(N-1)/2$  are shown in Fig. 8. We observe the EE in the gapped region ( $J < h$ ) is small until near the critical point, where it abruptly tends to become divergent as predicted by CFT [23, 24, 25, 26]. While in the gapless region ( $J > h$ ), we observe  $S_{(N-1)/2}$  with  $N \rightarrow \infty$  approaches its minimal value 2 when  $h \rightarrow 0$ . In fact, one can verify that  $|E_0^{(O,o)}\rangle$  evolves with  $h \rightarrow 0$  adiabatically into a superposition of all kink states in Eq. (56), whose EE is exactly 2. As a comparison, the EE of the well-known GHZ state is  $\log_2 2 = 1$ .

#### 4.6. Finite temperature properties in the gapless region

In the gapless region, the dispersed but neatly aligned lowest  $2N$  states, (39)-(42), dominate the system's properties at low temperatures ( $T \ll 4h/k_B$ ), where  $k_B$  is the Boltzmann constant. This fact facilitates us to work out some quantities at low temperatures based on the partition function

$$Z = \sum_{q \in q^{(O,o)} \cup q^{(O,e)}} e^{-\beta E_q}, \quad (75)$$

where  $\beta = \frac{1}{k_B T}$ . The DOS is defined as

$$\rho(E) = \frac{1}{N} \sum_{q \in q^{(O,o)} \cup q^{(O,e)}} \delta(E - E_q). \quad (76)$$

If  $N \rightarrow \infty$ , the summation in the 1st BZ can be replaced with integral, so we get a DOS,

$$\rho(x) = \frac{4(x + 2J - 2h)}{\pi \sqrt{x(x - 4h)(4h - x - 4J)(x + 4J)}}, \quad (77)$$

where  $x = E - E_0$ . It can be expanded as

$$\rho(x) = ax^{-1/2} + bx^{1/2} + O(x^{3/2}) \quad (78)$$

with

$$a = \frac{(J-h)^{1/2}}{\pi(Jh)^{1/2}}, b = \frac{(h^2 + Jh + J^2)}{8\pi(Jh)^{3/2}(J-h)^{1/2}}. \quad (79)$$

So we get the specific heat per site at low temperature,

$$\frac{C_M(T)}{N} \approx \frac{k_B}{2} \left[ 1 + \frac{2bk_BT(4a + bk_BT)}{(2a + bk_BT)^2} \right]. \quad (80)$$

## 5. Experimental proposal

We can design a large enough one to see the effect of ring frustration with nowadays state-of-art techniques based on laser-cooled and trapped atomic ions. In fact, the case for  $N = 3$  has been experimentally realized [7]. To generate a system with larger  $N \in \text{Odd}$  and ensure that the frustration comes from the ring geometry not from short-range interactions, we provide another proposal.

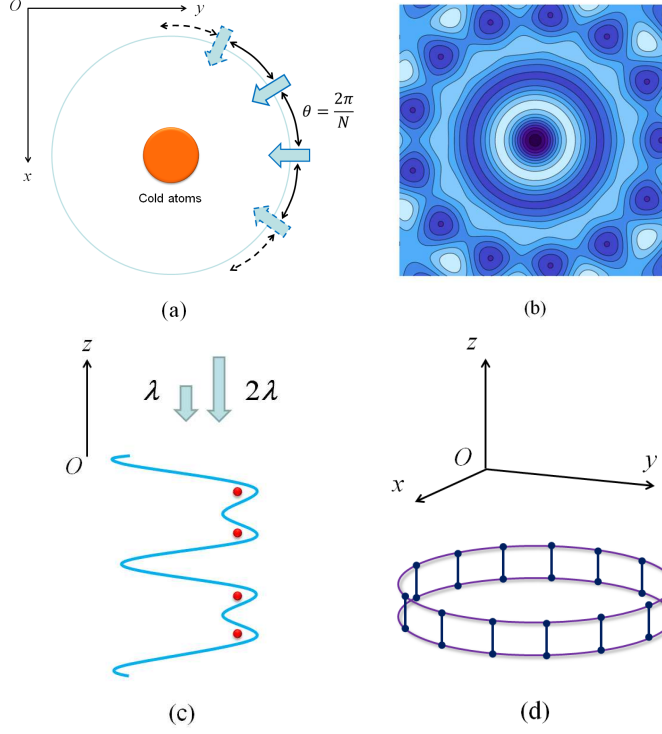
In our proposal as shown in Fig. 9, there are two key points. The first point is to produce a ring potential with odd number of traps. In  $x$ - $y$  plane, we impose  $N$  beams of independent standing wave lasers which are obtained by frequency selection. Then, each standing wave will contribute an optical potential along  $\vec{k}_i$  direction that can be expressed as  $V_{x-y} \cos^2(\vec{k}_i \cdot \vec{r}_i - \phi)$  for the  $i$ -th beam, where  $\vec{k}_i$  is the strength of beams and  $\phi$  is the phase shift. The angle between two neighboring lasers is  $2\pi/N$ . Thus, by adopting appropriate  $V_{x-y}$  and  $\phi$ , we can obtain a circular lattice potential with  $N$  traps in  $x$ - $y$  plane (Fig. 9(a) and (b)).

The second point is to realize the antiferromagnetic transverse model robustly. In  $z$  direction we apply two independent standing wave lasers,  $V_{z1} \cos^2(k_z z)$  and  $V_{z2} \cos^2(2k_z z)$ , where the former has twice wave length of the latter. Eventually, we obtain a periodical two-leg ladder potential by forming a double-well potential in  $z$  direction (Fig. 9(c) and (d)). In real experiment, there is additional harmonic trapping potential  $V_{trap}(x^2 + y^2)$ . The total potential can be written as

$$V(x, y, z) = V_{trap}(x^2 + y^2) + V_{z1} \cos^2(k_z z) + V_{z2} \cos^2(2k_z z) + V_{x-y} \sum_{i=1}^N \cos^2(\vec{k}_i \cdot \vec{r}_i - \phi). \quad (81)$$

Then, let us consider loading into the ladders with cold atoms which have two relevant internal states denoted as pseudo-spin states  $\lambda = \uparrow, \downarrow$ . The lattice potential experienced by cold atoms depends on which of those two internal states are located. For sufficiently deep potential and low temperatures, the system will be described by the following bosonic or fermionic Hubbard model [27],

$$H_{Hub} = \sum_{j,\lambda,s} (-t_\lambda) (a_{j\lambda,s}^\dagger a_{(j+1)\lambda,s} + \text{h.c.}) + \sum_{j,\lambda} (-t_\lambda) (a_{j\lambda,1}^\dagger a_{j\lambda,2} + \text{h.c.}) + \frac{1}{2} \sum_{j,\lambda,s} U_\lambda n_{j\lambda,s} (n_{j\lambda,s} - 1) + \sum_{j,s} U_{\uparrow\downarrow} n_{j\uparrow,s} n_{j\downarrow,s}, \quad (82)$$



**Figure 9.** (a) Scheme of the proposed experimental setup in  $x$ - $y$  plane. Each arrow depicts a wave vector of a standing-wave laser. The angle between any two neighboring lasers is  $2\pi/N$ . (b) The exemplified color map of optical potential where a ring of 13 trapping wells is shown by the dark blue potential wells. (c) The arrangement of lasers in  $z$  direction, where two standing wave lasers form an isolated double wells potential. (d) The total two-leg ladder potential.

where  $s = 1, 2$  is the leg index. With the conditions of Mott insulator limit  $t_\lambda \ll U_\lambda$ ,  $U_{\uparrow\downarrow}$  and half filling  $\langle n_{j\uparrow,s} \rangle + \langle n_{j\downarrow,s} \rangle \approx 1$ , the low-energy Hamiltonian of (82) is mapped to the XXZ model by second-order perturbation,

$$\begin{aligned}
 H_s = & \sum_{j,s} \pm J_\perp (S_{j,s}^x S_{j+1,s}^x + S_{j,s}^y S_{j+1,s}^y) + J_z S_{j,s}^z S_{j+1,s}^z \\
 & + \sum_j \pm K_\perp (S_{j,1}^x S_{j,2}^x + S_{j,1}^y S_{j,2}^y) + K_z S_{j,1}^z S_{j,2}^z,
 \end{aligned} \tag{83}$$

where the pseudo-spin operator  $\mathbf{S} = a^\dagger \vec{\sigma} a / 2$ ,  $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$  are the Pauli matrices and  $a^\dagger = (a_\uparrow^\dagger, a_\downarrow^\dagger)$ . The positive signs before  $J_\perp, K_\perp$  are for fermionic atoms and negative signs for bosonic one. The interaction coefficients for bosons are given by,

$$\begin{aligned}
 J_\perp &= \frac{4t_\uparrow t_\downarrow}{U_{\uparrow\downarrow}}, J_z = \frac{2(t_\uparrow^2 + t_\downarrow^2)}{U_{\uparrow\downarrow}} - \frac{t_\uparrow^2}{U_\uparrow} - \frac{t_\downarrow^2}{U_\downarrow}, \\
 K_\perp &= \frac{4t'_\uparrow t'_\downarrow}{U_{\uparrow\downarrow}}, K_z = \frac{2t'^2_\uparrow + t'^2_\downarrow}{U_{\uparrow\downarrow}} - \frac{t'^2_\uparrow}{U_\uparrow} - \frac{t'^2_\downarrow}{U_\downarrow}.
 \end{aligned}$$

For fermions, we only need to omit the last two terms in  $J_z$  and  $K_z$ . By modulating the intensity, the phase shift of the trapping laser beams, and the  $s$  wave scattering length through Feshbach resonance, we can obtain a desired Hamiltonian from (83),

$$H_s = \sum_{j,s} J_z S_{j,s}^z S_{j+1,s}^z + \sum_j K \vec{S}_{j,1} \cdot \vec{S}_{j,2}. \quad (84)$$

The properties of this system are dominated by the pseudo-spin singlet  $|s\rangle_j = (|\uparrow\downarrow\rangle_j - |\downarrow\uparrow\rangle_j) / \sqrt{2}$  and triplet  $|t_0\rangle_j = (|\uparrow\downarrow\rangle_j + |\downarrow\uparrow\rangle_j) / \sqrt{2}$  on the rung of the ladders in low energy. At this time, the system can be mapped to the transverse Ising ring, (1), that we desired [28].

## 6. Conclusion and discussion

In this work we have treated a special system, the transverse Ising ring, with perfect PBC. The main focus is placed on the case with ring frustration due to antiferromagnetic seam. We have demonstrated how the fermionic a-cycle problem is applied for solving the transverse Ising ring based on a method of band structure analysis. We have shown it is crucial to project out the redundant DOF of the fermions to restore the full DOF of the original spin model. The oddity of the number of lattice sites triggers or shuts the presence of ring frustration. The most intriguing result is that the system in strong antiferromagnetic region develops a gapless spectrum when the ring frustration is turned on no matter how large the system is. To the best of our knowledge, this gapless spectrum is totally unaware in previous investigations. The non-local nature of the longitudinal correlation function of the ground state is uncovered in detail. To understand all the fascinating properties of the system, we presented a treatment of perturbative theory for a simple but reliable cartoon picture of the formation of gapless spectrum. As an approximation for large enough system and low enough temperature, the DOS and specific heat are worked out. We also proposed an experimental protocol for observing the fascinating phenomenon due to the ring frustration.

There are some issues need to be specified. First, the method of band structure analysis encounters a problem for evaluating thermodynamic quantities at arbitrary temperature, because the fermionic a-cycle problem is not a free fermion one, to which the Fermi distribution can not be applied and the summation on the constraint fermionic states can not be accomplished in a closed form. But for finite system, it is just a matter of amount of computation. The finite system can be utilized to produce highly entangled states. Second, the method for the a-cycle problem can not be applied to the system with OBC, where the c-cycle problem is applicable.

The oddity-induced phenomenon is reminiscent of the one in the well-known spin ladders [29]. But the situation here is more dramatical because the difference between the consequences of  $N \in \text{Even}$  and  $N \in \text{Odd}$  is robust even when  $N \rightarrow \infty$ .

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**Appendix A. Proof of a Theorem**

*Theorem: Consider a Toeplitz determinant*

$$\Theta(r, N) = \begin{vmatrix} D_0 + \frac{2}{N} & D_{-1} + \frac{2}{N} & \cdots & D_{-r+1} + \frac{2}{N} \\ D_1 + \frac{2}{N} & D_0 + \frac{2}{N} & \cdots & D_{-r+2} + \frac{2}{N} \\ \cdots & \cdots & \cdots & \cdots \\ D_{r-1} + \frac{2}{N} & D_{r-2} + \frac{2}{N} & \cdots & D_0 + \frac{2}{N} \end{vmatrix} \quad (\text{A.1})$$

with  $D_n = \int_{-\pi}^{\pi} \frac{dq}{2\pi} D(e^{iq}) e^{-iqn}$ . If the generating function  $D(e^{iq})$  and  $\ln D(e^{iq})$  are continuous on the unit circle  $|e^{iq}| = 1$ , then the behavior for large  $N$  and  $r$  of  $\Theta(r, N)$  is given by

$$\Theta(r, N) = \Delta_r \left(1 + \frac{2\alpha}{D(e^{i0})}\right), \quad (\text{A.2})$$

where  $\alpha = \frac{r}{N}$ ,  $\Delta_r = \mu^r \exp(\sum_{n=1}^{\infty} n d_{-n} d_n)$ ,  $\mu = \exp[\int_{-\pi}^{\pi} \frac{dq}{2\pi} \ln D(e^{iq})]$ , and  $d_n = \int_{-\pi}^{\pi} \frac{dq}{2\pi} e^{-iqn} \ln D(e^{iq})$ , if the sum  $\sum_{n=1}^{\infty} n d_{-n} d_n$  is convergent.

*Proof:* Let  $e^{iq} = \xi$ ,  $D_n = \int_{-\pi}^{\pi} \frac{dq}{2\pi} D(\xi) \xi^{-n}$ . First, we rewrite Eq. (A.1) as

$$\begin{aligned} \Theta(r, N) = & \begin{vmatrix} D_0 & D_{-1} & \cdots & D_{-r+1} \\ D_1 & D_0 & \cdots & D_{-r+2} \\ \cdots & \cdots & \cdots & \cdots \\ D_{r-1} & D_{r-2} & \cdots & D_0 \end{vmatrix} + \begin{vmatrix} \frac{2}{N} & D_{-1} & \cdots & D_{1-r} \\ \frac{2}{N} & D_0 & \cdots & D_{2-r} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{2}{N} & D_{r-2} & \cdots & D_0 \end{vmatrix} \\ & + \cdots + \begin{vmatrix} D_0 & \frac{2}{N} & \cdots & D_{2-r} \\ D_1 & \frac{2}{N} & \cdots & D_{2-r} \\ \cdots & \cdots & \cdots & \cdots \\ D_{r-1} & \frac{2}{N} & \cdots & D_0 \end{vmatrix} + \begin{vmatrix} D_0 & D_{-1} & \cdots & \frac{2}{N} \\ D_1 & D_0 & \cdots & \frac{2}{N} \\ \cdots & \cdots & \cdots & \cdots \\ D_{r-1} & D_{r-2} & \cdots & \frac{2}{N} \end{vmatrix} \quad (\text{A.3}) \end{aligned}$$

Then we compose a set of linear equations

$$\sum_{m=0}^{r-1} D_{n-m} x_m^{(r-1)} = \frac{2}{N}, \quad 0 \leq n \leq r-1. \quad (\text{A.4})$$

These equations have an unique solution for  $x_n^{(r-1)}$  if there exists a non-zero determinant:

$$\Delta_r \equiv \begin{vmatrix} D_0 & D_{-1} & \cdots & D_{1-r} \\ D_1 & D_0 & \cdots & D_{2-r} \\ \cdots & \cdots & \cdots & \cdots \\ D_{r-1} & D_{r-2} & \cdots & D_0 \end{vmatrix} \neq 0. \quad (\text{A.5})$$

By Cramer's rule, we have the solution:

$$x_0^{(r-1)} = \frac{\begin{vmatrix} \frac{2}{N} & D_{-1} & \cdots & D_{1-r} \\ \frac{2}{N} & D_0 & \cdots & D_{2-r} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{2}{N} & D_{r-2} & \cdots & D_0 \end{vmatrix}}{\Delta_r} \quad (\text{A.6})$$

$$x_1^{(r-1)} = \frac{\begin{vmatrix} D_0 & \frac{2}{N} & \cdots & D_{2-r} \\ D_1 & \frac{2}{N} & \cdots & D_{2-r} \\ \cdots & \cdots & \cdots & \cdots \\ D_{r-1} & \frac{2}{N} & \cdots & D_0 \end{vmatrix}}{\Delta_r} \quad (\text{A.7})$$

$$x_{r-1}^{(r-1)} = \frac{\begin{array}{c} \vdots \\ \left| \begin{array}{cccc} D_0 & D_{-1} & \cdots & \frac{2}{N} \\ D_1 & D_0 & \cdots & \frac{2}{N} \\ \cdots & \cdots & \cdots & \cdots \\ D_{r-1} & D_{r-2} & \cdots & \frac{2}{N} \end{array} \right| \end{array}}{\Delta_r}. \quad (\text{A.8})$$

So we arrive at

$$\Theta(r, N) = \Delta_r + \Delta_r \sum_{n=0}^{r-1} x_n^{(r-1)}. \quad (\text{A.9})$$

For our problem,  $\Delta_r$  can be evaluated directly by using Szegő's Theorem, so we need to know how to calculate the second term in Eq. (A.9). Follow the standard Wiener-Hopf procedure [13, 19, 18], we consider a generalization of Eq. (A.4)

$$\sum_{m=0}^{r-1} D_{n-m} x_m = y_n, \quad 0 \leq n \leq r-1 \quad (\text{A.10})$$

and define

$$x_n = y_n = 0 \quad \text{for } n \leq -1 \quad \text{and } n \geq r \quad (\text{A.11})$$

$$\begin{aligned} v_n &= \sum_{m=0}^{r-1} D_{-n-m} x_m \quad \text{for } n \geq 1 \\ &= 0 \quad \text{for } n \leq 0 \end{aligned} \quad (\text{A.12})$$

$$\begin{aligned} u_n &= \sum_{m=0}^{r-1} D_{r-1+n-m} x_m \quad \text{for } n \geq 1 \\ &= 0 \quad \text{for } n \leq 0 \end{aligned} \quad (\text{A.13})$$

We further define

$$\begin{aligned} D(\xi) &= \sum_{n=-\infty}^{\infty} D_n \xi^n, \quad Y(\xi) = \sum_{n=0}^{r-1} y_n \xi^n, \quad V(\xi) = \sum_{n=1}^{\infty} v_n \xi^n, \\ U(\xi) &= \sum_{n=1}^{\infty} u_n \xi^n, \quad X(\xi) = \sum_{n=0}^{r-1} x_n \xi^n. \end{aligned} \quad (\text{A.14})$$

It then follows from Eq. (A.10) that we can get

$$D(\xi) X(\xi) = Y(\xi) + V(\xi^{-1}) + U(\xi) \xi^{r-1} \quad (\text{A.15})$$

for  $|\xi| = 1$ . Because  $D(\xi)$  and  $\ln D(\xi)$  is continuous and periodic on the unit circle,  $D(\xi)$  has a unique factorization, up to a multiplicative constant, in the form

$$D(\xi) = P^{-1}(\xi) Q^{-1}(\xi^{-1}), \quad (\text{A.16})$$

for  $|\xi| = 1$ , such that  $P(\xi)$  and  $Q(\xi)$  are both analytic for  $|\xi| < 1$  and continuous and nonzero for  $|\xi| \leq 1$ . we may now use the factorization of  $D(\xi)$  in Eq. (A.15) to write

$$\begin{aligned} P^{-1}(\xi) X(\xi) - [Q(\xi^{-1}) Y(\xi)]_+ - [Q(\xi^{-1}) U(\xi) \xi^{r-1}]_+ \\ = [Q(\xi^{-1}) Y(\xi)]_- + Q(\xi^{-1}) V(\xi^{-1}) + [Q(\xi^{-1}) U(\xi) \xi^{r-1}]_-, \end{aligned} \quad (\text{A.17})$$

where the subscript  $+$  ( $-$ ) means that we should expand the quantity in the brackets into a Laurent series and keep only those terms where  $\xi$  is raised to a non-negative (negative) power. The left-hand side of Eq. (A.17) defines a function analytic for  $|\xi| < 1$  and continuous on  $|\xi| = 1$  and the right-hand side defines a function which is analytic for  $|\xi| > 1$  and is continuous for  $|\xi| = 1$ . Taken together they define a function  $E(\xi)$  analytic for all  $\xi$  except possibly for  $|\xi| = 1$  and continuous everywhere. But these properties are sufficient to prove that  $E(\xi)$  is an entire function which vanished at  $|\xi| = \infty$  and thus, by Liouville's theorem, must be zero everywhere [13, 19]. Therefore both the right-hand side and the left-hand side of Eq. (A.17) vanish separately and thus we have

$$X(\xi) = P(\xi) \left\{ [Q(\xi^{-1})Y(\xi)]_+ + [Q(\xi^{-1})U(\xi)\xi^{r-1}]_+ \right\}. \quad (\text{A.18})$$

Furthermore,  $U(\xi)$  can be neglected for large  $r$

$$X(\xi) \approx P(\xi) [Q(\xi^{-1})Y(\xi)]_+. \quad (\text{A.19})$$

Consider the term  $[Q(\xi^{-1})Y(\xi)]_+$ , because  $Q(\xi)$  is a  $+$  function, so we can expand it as a Laurent series and keep only those term where  $\xi$  is raised to a non-negative power,

$$Q(\xi) = \sum_{n=0}^{\infty} a_n \xi^n = (a_0 + a_1 \xi^1 + a_2 \xi^2 + \cdots + a_{r-1} \xi^{r-1}) + O(\xi^r), \quad (\text{A.20})$$

and then

$$Q(\xi^{-1}) = a_0 + a_1 \xi^{-1} + a_2 \xi^{-2} + \cdots + a_{r-1} \xi^{1-r}, \quad (\text{A.21})$$

where we have neglected the term  $O(\xi^r)$  for large  $r$  for clarity. From Eq. (A.4) and Eq. (A.14), we have

$$Y(\xi) = \sum_{n=0}^{r-1} y_n \xi^n = \frac{2}{N} (1 + \xi^1 + \xi^2 + \cdots + \xi^{r-1}), \quad (\text{A.22})$$

thus

$$\begin{aligned} & [Q(\xi^{-1})Y(\xi)]_+ \\ &= \frac{2}{N} [(a_0 + a_1 + a_2 + \cdots + a_{r-1}) + (a_0 + a_1 + \cdots + a_{r-2}) \xi^1 + \cdots + a_0 \xi^{r-1}]. \end{aligned} \quad (\text{A.23})$$

From Eq. (A.9), Eq. (A.14) and Eq. (A.19), we have

$$\sum_{n=0}^{r-1} x_n^{(r-1)} = X(1) = P(1) [Q(1)Y(1)]_+, \quad (\text{A.24})$$

$$\begin{aligned} & [Q(1)Y(1)]_+ = \frac{2}{N} [r(a_0 + a_1 + a_2 + \cdots + a_{r-1}) \\ & - \frac{2}{N} [a_1 + 2a_2 + \cdots + (r-1)a_{r-1}] \end{aligned} \quad (\text{A.25})$$

$$= \frac{2}{N} \left[ rQ(1) - \frac{dQ(\xi)}{d\xi} \Big|_{\xi=1} \right]. \quad (\text{A.26})$$

So when  $r \gg 1$ , we can ignore the second term in Eq. (A.26). Together with Eq. (A.16), we get

$$X(1) = \frac{2r}{N} P(1) Q(1) = \frac{2r}{ND(1)} = \frac{2r}{ND(e^{i0})}. \quad (\text{A.27})$$

At last, by Szegő's Theorem, we get

$$\Delta_r = \mu^r \exp\left(\sum_{n=1}^{\infty} n d_{-n} d_n\right), \quad (\text{A.28})$$

where

$$\mu = \exp\left[\int_{-\pi}^{\pi} \frac{dq}{2\pi} \ln D(e^{iq})\right], d_n = \int_{-\pi}^{\pi} \frac{dq}{2\pi} e^{-iqn} \ln D(e^{iq}). \quad (\text{A.29})$$

From Eq. (A.9), we have

$$\Theta(r, N) = \Delta_r \left(1 + \frac{2\alpha}{D(e^{i0})}\right), \alpha = \frac{r}{N}. \quad (\text{A.30})$$

Q.E.D.

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